IV SUMMARY OF FINDINGS

The Panel's goals have been to note weaknesses that can be ameliorated through the use of more appropriate models and data, to seek clarification of the bases for certain of the analytical approaches and assumptions that have been used, and to evaluate the sensitivity analyses of alternative models and parameters.

A. Section II Findings -- TSPA Methodology

The Panel believes that the expectations for what TSPA can accomplish, as expressed in the "Methods and Assumptions" document, will not be achieved. Although the EPA standard (concerning a "reasonable expectation" requirement, quoted in Section II) no longer applies to the proposed Yucca Mountain repository, the explicit goals as expressed in these regulatory requirements are, in the Panel's view, more consistent with what the TSPA can achieve than are the goals that are stated in the "Methods and Assumptions" document.

Interpretation of TSPA Results

The TSPA-VA will inevitably be an uneven mixture of bounding analyses and of more realistic assessments. The point of noting this is two-fold. The first is to caution against overconfidence in the validity of the results of sensitivity analyses. Such results need to be interpreted with judgment, and recognized as being conditional on many assumptions [of varying validity]. The second point is to comment, as in our first report, on the issue of analyzability. The Panel's message is that for a repository to be licensable, it must be analyzable.

In this regard, the TSPA team needs to recognize that it may not be possible to analyze the impacts of certain postulated events on the performance of various systems and components. This applies, in particular, to the responses of various systems to potential events, such as volcanism and criticality, and the thermal pulse. It includes details such as how a waste package might degrade under impacts of this nature. This is a difficult and perplexing problem. Careful thought needs to be given to how it is to be addressed.

Although the Panel supports the "defense-in-depth" philosophy, there has been a tendency on the part of the Project team to judge the benefits of selected EBS/WP components with insufficient technical review of whether their contributions can actually be achieved. Without sufficient analysis or documentation to support the presumed performance, the resulting sensitivity analyses can be misleading. An unrealistic bounding analysis may, in some cases, indicate incorrectly that a particular feature of the site or design is unimportant to performance, while, in fact, it is important; an analysis that is unrealistically optimistic may mask the actual sensitivities in some aspects of the performance of that system and/or component.

Because of the inevitable and inherent uncertainties of the TSPA process, the DOE contractors must be prepared to explain the limitations of their analyses. Other groups who review this work will certainly point out the philosophical and practical limitations of the TSPA-VA.

Model Testing

On the basis of its review, the Panel has concluded that the TSPA team is not taking advantage of existing opportunities to test the validity of the models being used. To assist in correcting this problem, the Panel recommends that the Project team investigate methods by which subsystem models can be explicitly tested. These might include: (1) design of experiments to test specific results of the near-field models; (2) testing far-field models using the larger scale experiments in the Exploratory Studies Facility; (3) blind-testing of geochemical and hydrologic models in different geologic systems or localities; and (4) determination of whether the methodology used in the TSPA provides results that are consistent with natural systems. One such opportunity would be to use the existing models to predict the results/data that will be generated through the Drift Scale Test. Successful assessments based on careful analysis can provide substantial confidence in the TSPA analysis.

Use of Expert Elicitations

Overall, the Panel is impressed with the use of an advanced methodology for the conduct and interpretation of the expert elicitations. The Panel, however, continues to be concerned about the possibility that this process could be misused or abused by the Project team.

The value of expert elicitation is that in some situations, the elicitation process, involving interactions among the experts, can help resolve a lack-of-consensus situation. What an elicitation cannot accomplish is equally important: (1) it cannot develop "data" or a substitute for data where none exist; (2) while it can provide a mechanism for evaluating the existing data, it often cannot provide a means for successfully "assembling" them into a useful data set for the needs at hand; and (3) if the issue is to select from competing models to explain the relevant phenomena, rather than to understand differences among data sets of varying relevance, the interactions among the experts may not be able to resolve which among the several models is "best."

The Safety Case

While the TSPA addresses the likelihood, timing, and consequences of events and processes that could lead to a release of radioactive materials from the repository, a safety case looks at the same information and analyses with the objective of identifying the key features in why a repository could operate safely. Because the performance assessment and safety case share an underlying technical basis, the confidence that one can have in the TSPA results will, to a large degree, depend on how the analyses of the major elements of the defense-in-depth strategy are conducted and presented. These elements include the durability of waste form; canister lifetime; delays and limitations in the contact of water with the waste; and travel times to the repository boundaries, as either dissolved or colloidal species. They can be presented in a framework that includes the supporting models and their underlying physical and chemical principles, conformance with available laboratory and field data, experiences with similar models in comparable systems, and sensitivity analyses based on alternative plausible models. If this is done effectively, the principle of defense-in-depth will have been applied effectively.

Enhancing the Utility of the TSPA-VA

There are a number of actions that can be taken to enhance the utility of the TSPA-VA. Those considered important by the Panel include recognition of: (a) multiple objectives for the analysis (for example, to help DOE with its decision about whether to proceed to licensing, to identify data and analyses to improve future analyses and reduce their uncertainties, and to assist with design choices); (2) expectations for and limitations in what the TSPA-VA can do, (given the complex, coupled processes and long time periods of interest, it may not be possible to analyze the impacts of certain postulated events on the performance of various systems and components); and (3) the availability of tools to address the analytical limitations, for example, model testing, the appropriate use of expert elicitation, and defense-in-depth.

B. Section III Findings -- Technical Issues

Initial Conditions

The studies of radionuclide tracers (for example, ^{36}Cl) suggest that the discrepancies between the data and the conceptual models need further attention. This is a problem of considerable complexity and is beyond the scope of the charge to the Panel. Nonetheless it is extremely important. A prime example is the important role of the UZ flow model in the Yucca Mountain Project team's strategy as it approaches the license application phase.

Site Conditions with Waste Present

A number of models that can simulate the physics and chemistry of the governing processes have been developed. In particular, the response of the proposed repository has been analyzed at length under: (1) the current ambient conditions, and (2) the impact of a thermal perturbation. This has been an effort without precedent, and is complicated by the fact that adequate empirical evidence on the thermohydrologic, thermochemical and thermomechanical behavior in systems of this kind is not available. Under these circumstances, it is understandable that there will be uncertainties in the results that must be recognized and evaluated to the best possible degree.

Modeling studies have revealed significant differences in the potential effects of the thermal field on the hydraulic behavior of the repository system as the input value for the infiltration rate was varied from the previous estimate of 0.1 mm/year to the currently estimated rate of 4.4 mm/yr. It is apparent that the magnitude of this critical factor must be well established, so that the potential effects on repository behavior can be accurately evaluated.

Fracture/matrix interactions play a dominant role on the infiltration rate. In the coarse grid simulation, these interactions are simulated through the use of effective parameters, such as the area between the fractures and matrix. This is currently expressed by a reduction factor to reflect the limited contact resulting from channelized fracture flow. Reduction factors as low as 10^{-3} have been postulated to match field data. This is a drastic departure from the simulation practices previously used. At the present time, the foundation for this factor is weak. Additional uncertainty, particularly for two-phase flow processes (imbibition, drainage and heat pipes), is introduced through the use of volume averaging over a number of fracture-matrix areas. In such cases, the set of hydrologic parameters applied will not correspond to that of either individual fractures or matrix blocks.

The TSPA team is using the equivalent continuum model (ECM) to assess the long term impacts of the thermal perturbation on the proposed repository. Application of this model requires that thermodynamic equilibrium exists between fracture and matrix. Although this may be true for thermal energy and for the imbibition of a high-permeability tuff, it will not necessarily be true for mass diffusion and imbibition of a low-permeability tuff, such as that at Yucca Mountain. ECM also cannot account for a fracture/matrix reduction factor, and this model is therefore inherently unable to match the revised percolation flux. Nonetheless, the ECM is being used extensively in evaluations of the thermohydrologic behavior of the proposed repository. This is of concern to the Panel and it has recommended steps that should be taken to assess uncertainties in and range of validity for how the ECM is being used.

Modeling studies have shown that volume changes are possible as a result of dissolution in the condensation zone, formation of secondary minerals, and the involvement of the fracture and matrix in the chemical evolution. Experimental studies have shown that hydrothermal processes can alter minerals and cause them to precipitate at the fracture/matrix interface. The extent to which such reactions can lead to significant changes in the porosity and permeability of the rock system is a major uncertainty at this point. Laboratory investigations indicate that processes of this nature could significantly reduce the permeability of the fractured tuff. This may have significant implications on repository performance.

Engineered Barriers and Waste Package Performance

Reducing uncertainty

Large volumes of water will be mobilized by the thermal pulse. However, the flow paths and amounts of water transported along various paths are not well defined. This leads to large uncertainties in estimates of the amounts and distribution of seepage that would flow back into the drifts within the proposed repository. The spatial and temporal characteristics of these flows are also uncertain. The impacts of these uncertainties on overall repository performance can be reduced, and the reliability of the TSPA-VA increased, by the selection of highly corrosion resistant metals for the waste packages. For these reasons, the Panel supports a TSPA analysis that is based on the selection of the most corrosion resistant metals for the corrosion resistant metal barrier.

A steel outer barrier has several desirable features that pertain during a long, dry period. When wetted, however, the steel canister corrodes rapidly and adds to uncertainty. Dual packages comprised of a double layer of corrosion resistant metals have been proposed and are worthy of further consideration and evaluation in the performance assessment.

Improving information and data quality

Although notational information is available, there is a paucity of experimental data on the behavior of the alloys of interest in the environments anticipated to be present within the repository. Realistic data are needed to support the selection and evaluation of the performance of such materials. For this reason, the Panel recommends that a comprehensive effort be undertaken to compile and critically review the corrosion behavior of the two primary candidates for the corrosion resistant metal. These reviews should be directed to the class of alloys, not to a specific metal designation.

Analytical approach

The Panel concurs with the conclusion of the Waste Package Expert Elicitation effort, namely that crevice corrosion is the most important degradation mode to be considered in the TSPA-VA. With respect to stress corrosion cracking (SCC), the Panel notes that no mechanistic models are available for the TSPA-VA. Rather than suggest that resources be directed to additional model development, the Panel recommends that an engineering approach be applied, namely, that the Project team select metals that are resistant to SCC and specify design and manufacturing procedures that avoid SCC.

The need for and extent of galvanic protection will depend upon the geometry of the galvanic couple which, in turn, will depend on the nature of the perforation of the outer barrier and exposed area of the inner barrier, the presence or absence of corrosion products and deposits, and the chemical composition of the waters present. The basis for any credit assumed to be provided by galvanic protection, and how this is incorporated into the TSPA-VA, will need to be explicitly presented.

An extended dryout period resulting from the heat output from the waste packages is a basic feature of the current design. The thermal pulse will not be uniform due to variations in the waste packages and their placement, unused or unusable areas within the repository, and edge effects around the repository. As in the findings with respect to other aspects of the proposed repository, the conceptual description of the response of the waste packages to this large and nonuniform thermal pulse is not well developed.

Water chemistry

The chemistry of heated water has been modeled but there are limited experimental data for evaluating the models that have been developed. Unfortunately, the estimates generated using the current models do not correlate well with the experimental observations. As a result, the impacts of various factors on the chemistry of water entering or within the drifts remain an area of major uncertainty. The current project strategy and activities are unlikely to resolve these problems. The determination of water chemistries once a package has been penetrated is even more uncertain**.** More laboratory and field data on water chemistry, gathered under realistic conditions, are required to refine and validate the existing models.

Transport from the Engineered Barrier System

The conceptual description of transport from the EBS is poorly developed. A critical factor is the form and amount of water transport into and from waste packages that are assumed to be perforated. There are major uncertainties regarding: (1) the number and distribution of penetrations through the packages; (2) the morphology of the penetrations; (3) the presence or absence of corrosion products or deposits within the penetrations; (4) the form and composition of corrosion products/deposits outside the penetration; and (5) the form and composition of the waste form, transformation products and other materials within the package.

Treatment of Backfill

It is the understanding of the Panel that the base case for the TSPA-VA will be the “no backfill” case. Nonetheless, the Panel also understands that backfills of various types are under active consideration by the Project team. As a result, the Panel recommends that, so far as possible, an analysis of the backfill case be included in the TSPA-VA.

Glass Waste Form Degradation and Radionuclide Release

The decision to use a response surface for the description of glass degradation and release fails to take into account an enormous amount of relevant published laboratory data, the variety of existing conceptual models for glass dissolution, and studies of natural analogues of glass dissolution that have been developed over the past twenty years. For these reasons, the Panel anticipated that the TSPA-VA team would include a rigorous comparison of these data sets to the modeled response surface. This does not appear to be the case. Although the response surface approach may be computationally efficient, mechanistic models would provide a stronger basis for long-term extrapolations of glass dissolution.

It is not clear to the Panel how models, which only have pH and silica concentration as their principal parameters, can be used to calculate solubility limits for phases that form during the alteration of glass. The model used to describe the dissolution of the glass waste forms also does not account for concentrations of chemical species (for example, the ferric ion) in the corroding solutions which may enhance the leach rates. In addition, the present model does not explicitly include estimates of the vapor phase alteration of glass.

One of the important issues identified over the past few months is the time dependent evolution of solution compositions and the structure and composition of the alteration/gel layer on the surface of corroded glass. The gel layer is now viewed as important because it can either be an efficient "sink" for rare earth elements and actinides or a source of colloids with high actinide concentrations. The potential retardation of actinides in this layer may justify a more sophisticated approach, that is, one that considers the role of the gel layer.

Prior to the breach of containers and contact with water, glass will experience an extended thermal pulse and be subjected to high fluxes of ionizing radiation. The TSPA team should evaluate whether there are any deleterious effects on the glass waste form as a result of the combined effects of these stresses. As in the other studies, the full range of types of glass waste forms anticipated to be placed in the repository need to be considered.

Disruptive Events, Criticality, and Climate Change

Volcanism

If the probabilities of the occurrence of volcanic events are so low as the hazard analyses indicate, the Project team should be able to screen out volcanism from consideration in the performance assessment on input-frequency grounds alone. If this proves to be the case, extensive work on the potential effects of various volcanism scenarios would not be necessary.

Inadvertent Human Intrusion

Given the uncertainty in what the regulatory bodies will ultimately adopt, the approach that the TSPA-VA team is taking at this time appears to be eminently sensible.

Criticality

The Panel believes that the two key elements of the approach of the TSPA team for the analysis of criticality -- allowing criticality to be studied through side analyses instead of in the mainline TSPA modeling, and developing a few scenarios for analysis in order to bound the problem -- are both sensible. The Panel commends the Project team for the logic adopted in the work being undertaken. If the consequences of criticality are so low as to make it unimportant, then the question of its analyzability may become moot.

Transport

Colloids

Evidence has recently been reported of the colloidal transport of radionuclides (^{60}Co, ^{137}Cs, Eu, and Pu) through fractured volcanic rock at the Nevada Test Site (NTS). The Panel recommends that these data be carefully analyzed to determine their applicability to the TSPA. The Panel also recommends that data available at other locations within the NTS be used to evaluate the models that have been developed to describe radionuclide transport within the proposed Yucca Mountain repository.

Biosphere and Dose

It is possible that the U.S. EPA and the USNRC will provide the Project team with specific values for the dose conversion factors and risk coefficients that are to be used in the TSPA-VA. Even so, the DOE and the Project team should seek to gain an understanding of the conservatisms that underlie, and have been incorporated into, these factors. It is also important that the team recognize additional conservatisms that may result from the use of the concept of the committed dose and the assumption of a linear dose response relationship. For these and other reasons, the Panel does not agree that the process of estimating the doses and risks from radionuclide concentrations in groundwater, and other media, is as “simple” as implied by the TSPA team. In making this recommendation, however, the Panel wants to make it clear that it is not seeking to imply that the TSPA-VA team should develop new more realistic dose conversion factors and risk coefficients; rather it is to encourage the TSPA-VA team to be aware of these conservatisms, to quantify them at least in a cursory sense, and to be prepared to discuss and evaluate their implications in terms of the outcome of the TSPA-VA.

Procedures used for identifying the critical radionuclides need to be carefully reviewed. The Panel notes that the NCRP has concluded "that ^{129}I does not pose a meaningful threat of thyroid carcinogenesis in people." These types of issues should be analyzed and discussed with the regulators to ensure that there is a scientifically sound basis to support whatever regulations are adopted. Similar reviews should be conducted of the detailed physical, biological, and chemical information on each of the other radionuclides considered important by the TSPA-VA team. The goal should be to define a sound scientific basis for the selection of each such radionuclide.

APPENDIX A: The Fracture-Matrix Interaction: Reduction of Uncertainty

The fracture-matrix interaction: Reduction of uncertainty

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Submitted to the Review Panel of TSPA-VA, October 31, 1997

Summary

A good description of the fracture-matrix interaction is necessary to reduce uncertainties in the numerical predictions of the repository performance and in process assessment, in general. In many cases, this interaction takes the simple form of a competition between advection in the fracture network and diffusion (mass, heat, capillarity) in the matrix. The partition of flow between fracture and matrix is dictated by parameters such as the capillary diffusivity (imbibition), the area of interaction and the amount of maximum trapped saturation of the non-wetting phase (air) in the grid block volume. Reaching conditions of fracture-matrix equilibrium is controlled by the magnitude of the diffusivity, the flow rate partition and the time elapsed. In typical applications, fracture-matrix equilibrium is likely for thermal energy and for the imbibition of a high-permeability matrix, but unlikely for mass diffusion and the imbibition of a low-permeability tuff. The latter is common to many rocks of the Yucca mountain. In such cases, the assumption of equilibrium is likely to fail. In the current coarse grid simulation, the representation of this interaction is through effective parameters, notable among which is the effective area of fracture-matrix interaction, expressed through a reduction factor that reflects the limited contact resulting from channelized fracture flow. To match field data, reduction factors as low as 10^{-3} have been postulated. This is a drastic departure from previous simulation practice, where this concept was not used. Additional uncertainty, particularly for two-phase flow processes (imbibition, drainage and heat pipes), is introduced due to the volume-averaging over a number of fracture-matrix areas, inherent to the coarse description.

Main recommendations that may help reducing this uncertainty include:

1. <u>Revisit the concept of reduction factor</u>.

Use the experimental information reported in Glass et al. (1997) and earlier publications, on displacement patterns at various conditions, to estimate reliably the effective area (and the corresponding reduction factor). Then, account for a possible increase of the factor due to the stabilization of the displacement exerted by imbibition in the matrix. Modify the fracture hydrological parameters, particularly the relative permeabilities, to account for channelized displacement, by considering rate and gravity effects where appropriate. Allow for anisotropy in permeability, displacement and reduction factor in the fracture continuum in the horizontal and vertical directions.

2. <u>Allow for the possibility of non-zero trapped (residual) air saturation</u>.

Account for non-zero trapped saturation in the various lithological units, by considering the direction (imbibition) and rate of invasion. Consider the effect of large-scale trapping, due to large-scale heterogeneity in the grid block, in increasing the effective residual gas saturation. Non-zero values may lead to lower, and thus more defensible, reduction factors.

3. <u>Improve the estimation procedure for matching field hydrologic data</u>.

Analyze the limitations of the 1-D model (only vertical flow) currently used to match field data and estimate parameters. Allow for the possibility of lateral flow, due to capillary and flow barriers, anisotropy, etc. Study the consequences of non-uniqueness inherent to the inversion process.

4. Improve the large-scale description of two-phase flow processes.

Revisit the formalism for representing unsaturated flow in a grid block, by accounting for effective large-scale permeabilities, relative permeabilities, capillary pressures, large-scale trapped saturations and the fracture-matrix interaction. In this context, particular attention needs to be payed to the heat pipe description in this context. Consider the extension of the particle-tracking algorithm to 3-D and to other diffusive processes.

5. Justify the use of ECM for TH predictions.

Carefully delineate the validity of capillary equilibrium in ECM applications. Revisit the ECM formalism and validity in light of 1 and 2 above. Revisit the heat pipe representation.

Other recommendations are listed in the text.

The fracture-matrix interaction: Reduction of Uncertainty

The ultimate criteria for the viability assessment of the Yucca Mountain repository are the arrival times and the concentrations of potentialy released radionuclides to the biosphere and the accessible environment. These are determined by two different processes:

- The rates of release of radionuclides from the site- due to the breaching of its integrity by corrosion.

- Their transport from the repository to the accessible environment.

Both processes depend crucially on the distribution of liquid and gas flows in the mountain. The potential for canister corrosion, thus the release rate, is a function of the humidity at the repository, which is dictated by the fluid flow distribution in the mountain, in response to infiltration and the heat released from the spent fuel. In radionuclide transport, advection by flow is the predominant mechanism and controls transport rates, even at the relatively small expected infiltration rates (order of mm/year).

In such a problem, to quantitatively formulate a criterion requires:

- (i) a qualitative (physical) understanding of the factors affecting flow and transport in the subsurface;

- (ii) a characterization of the subsurface (initial conditions) and of the infiltration rates (boundary conditions) with acceptable (or at least bounded) uncertainty; and

- (iii) a mathematical (numerical) model of acceptable (or at least bounded) accuracy.

A major factor that hampers the reduction of uncertainty is the heterogeneity in subsurface properties, a basic component of which in Yucca mountain is its extensive fracturing. In this report, we will focus on this important factor, and specifically on the *fracture-matrix interaction*, in the context of the three issues noted above.

(i). Physics

In connection to the repository performance, the main physical processes of interest are:

- transport of molecular species (e.g. potentially released radionuclides or colloids)

- transport of thermal energy (due to the released heat from the waste), and

- transport of multiphase momentum, the latter being mostly imbibition from rain infiltration (drainage is also discussed below)

In the fractured mountain, these three transport processes occur by essentially similar mechanisms: mostly by advection in the fractures, and mostly by diffusion in the matrix, where fluid flows are relatively slow (see also below). Matrix diffusion includes diffusion of molecular species, heat conduction, or capillary imbibition, in the respective cases. Although different from one another (for example, imbibition is a non-linear process, it is history-dependent, it may involve additional non-diffusive phenomena, etc.) they all share common diffusive aspects. Transport is also influenced by retardation, for example the sorption of molecular species in the matrix (particularly when the formation is zeolitized), of heat in the rock matrix, or by the filtration of colloidal particles mostly in the fractures.

The transverse transport from fracture to matrix originates at the fracture-matrix boundary (see schematic of Figure 1). Thus, its rate will be influenced by the effective area of contact between fracture and matrix. We note in advance that this area is not necessarily the entire geometric fracture-matrix interface, but can be only a fraction of it (for example, when fluid flow in the fracture is channelized). The fracture-matrix interchange will also be affected by the competition between advection and diffusion. These issues are extensively discussed below.

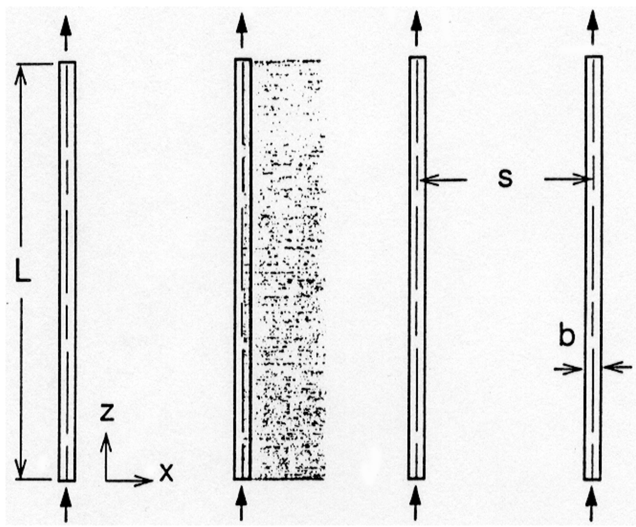

Figure 1. Simplified schematic of the fracture-matrix interface. (From Zyvoloski et al. (1997)).

The fracture-matrix interaction is fundamental to the determination of the flow distribution and transport rates, at conditions of saturated or unsaturated flow. Consider, for example, saturated (single-phase) flow. In the absence of any fracture-matrix interaction, transport will occur either in a well-connected fracture continuum of porosity ϕ_f, or in a well-connected matrix continuum of porosity ϕ_m. Assuming that the same overall amount of fluid flows in each, and that transport is dominated by advection, the ratio of the respective arrival times of an advected quantity (mass, heat, etc.) is simply

$$\frac{t_m}{t_f} = \frac{\phi_m}{\phi_f} \tag{1}$$

For typical values in the Yucca mountain, this is of the order of 100-1000 (see also Figure 2 below). When single-phase flow occurs in parallel in both the matrix and the fracture network, the ratio of fluid velocities in the fracture and the matrix, therefore the ratio of arrival times in the matrix to the fracture (again in the absence of diffusion), is

$$\frac{t_m}{t_f} = \frac{k_f}{k_m} \tag{2}$$

where k is permeability. For typical values in the Yucca mountain this ratio can be of the order of 100,000. On the other hand, in the limit when diffusion in the matrix is very strong (with a criterion to be developed below), such that fronts advance in the matrix and fracture continua at the same rate, the corresponding ratio in arrival times would be of order 1. Parenthetically, the latter is essentially a condition of *equilibrium* between matrix and fracture, and forms the basis of the widely used ECM model (see discussion below).

These simple examples show the great disparity in predicted arrival times depending on the assumed degree of the fracture-matrix interaction and the competition between advection and diffusion. Such disparity has been observed in the particle transport simulations of Robinson et al. (1997), where arrival times can vary in the range 10 years to 10,000 years. Correspondingly, depending on the strength of diffusion (heat conduction, capillarity), an analogous disparity may also apply to temperature and fluid distributions, as discussed below. In reality, arrival times will also be affected by many additional factors, such as the dispersion of flow paths in a single fracture (due to aperture variability and correlation), in the fracture network (due to branching of fractures or fracture termination or other causes of poor fracture connectivity) and in the matrix (due to permeability heterogeneity), by the strength of the diffusive process, by retardation, by conditions of unsaturated flow and by the effective area of contact between fracture and matrix. In this report, the factors pertaining to the fracture-matrix interaction will be emphasized.

Consider, first, the competition between advection and diffusion. For the case of mass and heat transport, this is expressed in terms of the Peclet number

$$Pe_i = \frac{qL}{D_i}; i = M, T \tag{3}$$

where M and T stand for mass and thermal energy respectively, D_i is the respective diffusion coefficient and L is a characteristic linear size. In the absence of restricted diffusion effects, mass diffusivity in the matrix is proportional to the species diffusivity D

$$D_M = \frac{\phi_m D}{\tau} \tag{4}$$

where τ is a tortuosity factor. Estimated typical values of D_M for transport in the liquid phase. are of the order of 10^{-10}-10^{-11} m^2/sec. (However, one must exercise caution in using this expression in very tight porous media, for example the heavily zeolitized tuff of Yucca Mountain, where diffusion will be restricted.) Thermal diffusivity in the matrix is substantially greater than mass diffusivity,

$$D_T = \frac{\lambda_H}{\rho C_p} \tag{5}$$

where λ denotes thermal conductivity and ρC_p, is volumetric heat capacity. For Yucca mountain conditions, a typical estimate of D_T is of the order of 10^{-7}-10^{-6} m^2/sec, which is three to four orders of magnitude greater than mass diffusivity in the liquid.

Diffusion control in the matrix requires that the Peclet number is smaller than unity. This can be accomplished at low velocities. For example, assuming L = 1 m (order of magnitude of the matrix block), mass transport in the matrix will be diffusion-controlled for velocities lower than about 3.1 mm/year. Given that this is of the order of magnitude of the currently accepted infiltration estimates and that most of the flow will actually occur in the fracture, diffusion control in the matrix is very likely. A similar dimensionless number can be defined to characterize the interaction between fracture and matrix: Assuming advection control in the fracture and diffusion control in the matrix, the competition between these two mechanisms can be expressed through the Peclet number

$$Pe_{i,f} = \frac{q_f l}{D_i}; i = M, T \tag{6}$$

where l is the matrix block size (of the order of 1 m for Yucca mountain). This number will be used below to assess the validity of the ECM model.

Consider, next, imbibition in an unsaturated matrix of a wetting liquid flowing in a saturated fracture, which is driven by the difference in the capillary pressure in the matrix and the fracture. This problem is more complex, since the flow of water and the water saturations will affect both diffusion (imbibition) in the matrix and advection. Under conditions of countercurrent flow, or if the overall fluid flow rate in the matrix is small, matrix imbibition can be approximated as nonlinear diffusion with a diffusion coefficient

$$D_c = -\frac{\phi_m k_m k_{rw}}{\mu}(dP_c / dS) \tag{7}$$

where S is liquid saturation, dP_c/dS is the slope of the capillary pressure curve at the particular saturation and μ is liquid viscosity. Since the capillary pressure is inversely proportional to the square root of the permeability by the Leverett expression, $P_c \sim \frac{\gamma}{\sqrt{k/\phi}} J(S)$ where γ is the inter-facial tension between gas and water, equation (7) gives an estimate of the magnitude of capillary diffusivity during imbibition

$$D_c \sim \frac{\gamma \phi_m^{3/2} \sqrt{k_m}}{\mu} \tag{8}$$

For example, for $\phi_m = 0.1$ and a TS tuff value of $k_m = 1$ μ d (=10^{-18} m^2/sec), a value of 1.8 x 10^{-9} m^2/sec is predicted, while for a much more permeable rock with $k_m = 1$ d (=10^{-12} m^2/sec), the diffusivity is about 1000 times larger. Thus, capillary diffusivity depends significantly on permeability and can be of the same order of magnitude as mass diffusivity in a liquid for tight rocks or as thermal diffusivity for very porous rocks. The rather sensitive dependence of imbibition on k underscores the importance of pore-lining minerals at the matrix-fracture interface, which will act to retard matrix imbibition (and essentially restrict the fracture-matrix interaction). Although superficially analogous to mass diffusion, however, it must be also noted that imbibition is a nonlinear process and that diffusivity will change as a function of saturation and of the history of imbibition (namely whether it is primary or secondary), through the variable $k_{rw} dP_c / dS$. For example, near dry conditions (expected during re-wetting of the repository rock at the conclusion of boiling), the latter is the product of a vanishing quantity, k_{rw}, multiplied by a quantity that diverges, dP_c / dS. This shows the importance of as accurate a determination of the hydrologic matrix properties as possible.

Some simple conclusions follow: Transport in the fracture will be mostly by convection, and in the matrix mostly by diffusion (compare with (1) and (2) above). Thermal equilibrium between matrix and fracture will be set in long before mass or capillary (for the case of tight rocks) equilibrium. A thin layer of pore-lining minerals is sufficient to reduce transverse diffusion into the matrix for the case of molecular species (due to low porosity) or imbibition (due to low permeability), but not for the case of thermal energy, the conduction of which occurs mostly over the solid matrix.

Assuming advection control in the fracture and transverse diffusion control in the matrix, a simple model can be used to study the effect of diffusion on arrival times during transport. Figure

2 from Zyvolvoski et al. (1997) shows results using such a simple model for the geometry of Figure 1. (An analogous model for heat conduction was used earlier by Lauwerier, 1955, and by Yortsos and Gavalas, 1982.) In this figure, GWTT ($= L/q_f$) is the convective time in the fracture, where L is the extent of the fracture while S is the fracture spacing (equal to l above). The figure shows the retardation in the arrival times as a result of transverse diffusion in the matrix and can also be used to infer the conditions for fracture-matrix equilibrium (as discussed below). Note that the upper limit in the vertical axis is ϕ_m / ϕ_f. Using our notation, the horizontal and vertical axes in the figure are $\left[\frac{Pe_{i,f} l}{L}\right]^{-1/2}$ and $\frac{Pe_{i,f} l}{L}\frac{TD}{l^2}$, respectively.

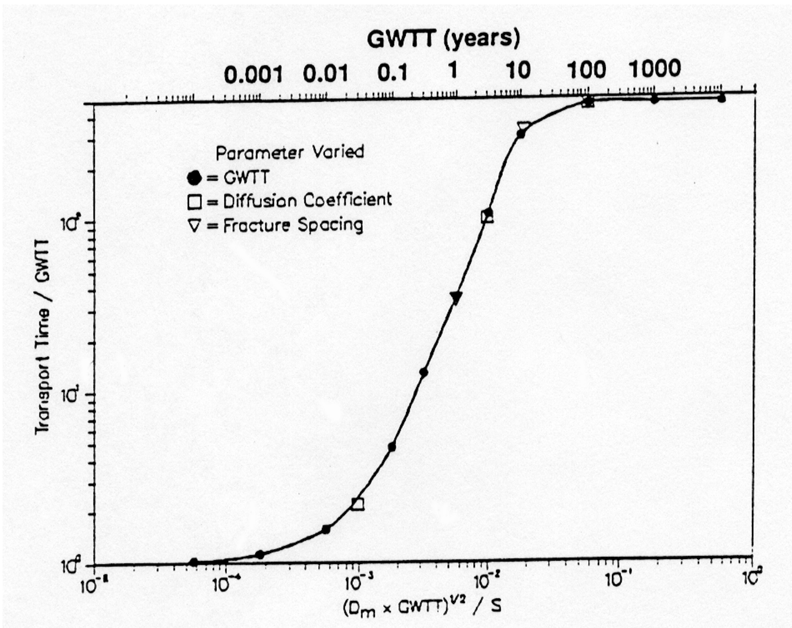

Figure 2. Arrival time for the transport of a tracer advected in the fracture and diffusing in the matrix. (From Zyvoloski et al., 1997.)

Conditions of saturated flow in the fracture (and in the matrix for that matter) will exist in the SZ far below the repository. However, in the UZ, all processes will be controlled by two-phase flow. Here, the direction of displacement is important and one needs to distinguish between drainage (in which the vapor phase, in the present context, displaces liquid), imbibition (which is the inverse process), and countercurrent flow (which will be present in heat pipes), as well as between primary and secondary drainage/imbibition. In the majority of instances in the Yucca mountain, the process of interest is secondary imbibition, resulting from water infiltration or from the condensation of vaporized liquid. However, drainage will also occur, specifically during the vaporization of liquid water near the emplaced waste. In addition, if completely dry conditions develop in the heated rock near the repository, the re-wetting of rock at the conclusion of the heating cycle will be primary imbibition, with much slower rates of matrix penetration. Finally, countercurrent flow will occur in heat pipes near the emplaced waste. The fracture-matrix interaction is a key factor dictating the distribution of fluids (hence the transport) under all these conditions.

During drainage, the non-wetting phase (e.g. the vapor) will remain in the fracture if its flow rate is not sufficiently high. Matrix penetration requires that the capillary entry pressure of the matrix (which scales as $\gamma / \sqrt{k_m}$) be exceeded. Such pressure difference can be provided by viscous (or gravity) forces in the matrix (see Haghighi et al., 1994). Under the conditions of Yucca mountain rates, however, this is rather unlikely. Thus, during drainage (e.g. boiling) the vapor phase will be present in the matrix only as a direct result of vaporization of the liquid in the matrix (and not by invasion from the fracture side). One should also recall in the present context, that vaporization of a liquid in a tight matrix requires an elevated boiling point, due to the porespace curvature (Kelvin effect). The roles of vapor phase diffusion as well as vapor flow, in this context, could also be important, but they will not be discussed here.

Whether at conditions of drainage, imbibition or countercurrent flow, the fracture-matrix interaction will also be affected by viscous and gravity forces, which play an important role in setting displacement patterns in the fracture. Consider the downwards displacement of gas by liquid in a single fracture isolated from (non-communicating with) the porous matrix. This displacement will be subject to the destabilizing effect of gravity, the stabilizing effect of viscous contrast and capillarity and the channeling in the fracture, if the aperture of the latter is spatially correlated (as it appears to be in many natural systems). The combination of these three factors will result in a fingered displacement in the fracture (see, for example, the work of Glass et al. summarized in Glass et al., 1996, 1997). Likewise, a fingering pattern will emerge in the upwards displacement of liquid by gas (for example during boiling), where now viscous instability will further promote the fingering pattern.

Fingering or channeling in the fracture will restrict the *effective area* between the fingered phase in the fracture and the matrix, therefore it is a key parameter of the fracture-matrix interaction. Depending on the extent of the correlation length, the capillary number, $Ca = \frac{q\mu}{\gamma}$, and the Bond number, $B = \frac{\Delta\rho g_x k_f}{\gamma}$, such fingering will not be amenable to the standard continuum description, e.g. using van Genuchten or Corey-Brooks parameters. Instead, rate and gravity effects (through *Ca* and *B)* and the correlation structure, must be included in its description. This problem has not yet been solved. However, we expect that the conventional approach currently used will start losing validity when *Ca* or *B* become larger than about 10^{-5}. This is likely for typical flow parameters (for example for water-air in a fracture of permeability 10^{-10} m^2, $B \sim 10^{-4}$). In addition, when infiltration is episodic, the flow may not necessarily occur continuously, but rather in the form of individual blobs of a finite extent. Fingering and channeling may also occur in the adjacent matrix. However, due to the relatively small amount of flow rate partitioned in the matrix, and the small matrix permeability, *Ca* and *B* will be sufficiently small, so that the continuum theory is expected to be applicable there.

We must note that if communication between matrix and fracture is allowed, imbibition of wetting liquid in the matrix block will act to reduce the severity of fingering. This problem is analogous to the stabilizing effect that heat losses to the adjacent formations have on the stability of a steam front during steam injection in a porous medium (Yortsos, 1982). The competition is essentially the same to that of advection vs. diffusion discussed above, and will depend on the flow rate in the fracture and the capillary characteristics of the matrix (or, essentially, on an equivalent Peclet number). To our knowledge, this problem has not been studied yet. (A different version of the same problem, but in a 2-D geometry, in which the fracture is essentially a line and fingering is not an issue, was studied by Nitao (1992), who showed the existence of a critical flow rate, q^*, above which the propagation of an advancing front in the fracture is faster than in the matrix. Essentially, Nitao 's criterion is equivalent to requesting that the process operates at the rightmost part of Figure 2 (see also discussion below regarding ECM). Pore-network simulations by Haghighi, 1994, have confirmed the existence of such transition).

When the unsaturated flow involves saturated steam (for example during boiling), steady-state heat pipes will be possible, in which there is countercurrent flow of vapor and liquid. Above the repository, vapor will move upwards, cool and condense, condensed liquid will move downwards, become heated and evaporate. Below the repository, the direction of flow is reversed. The mechanics of 1-D heat pipes are well understood, even though the precise mechanism for countercurrent relative permeabilities is not. However, in the Yucca mountain this process takes place in a fractured system. In such a system it is very likely that the vapor flow will be restricted only in the fractures, for the reasons described above. However, the return flow of liquid can be either in the matrix or in the fracture. Identifying the appropriate mechanisms and the effective fracture-matrix interaction will affect the calculation of the heat pipe extent, hence that of the dryout region.

It should be pointed out that a reduction of the effective interfacial area between fracture and matrix is possible even under conditions of saturated flow, provided that the fracture aperture distribution is heterogeneous and spatially correlated. In such cases, most of the fluid flow will take place over a backbone consisting of the largest connected apertures (e.g. see Katz and Thompson, 1986, Moreno and Tsang, 1994, Shah and Yortsos, 1996 for the corresponding porous media problem), thus diffusion into the matrix will, at least initially, occur from a substantially smaller area. This area will increase as a function of time, however, as transverse diffusion in the fracture will eventually spread the diffusing species over the entire fracture area.

(ii). Characterization

From the above it follows that the accurate characterization of the fracture-matrix interaction requires information on:

1. The hydrological characteristics of single fractures, including aperture statistics and its spatial correlation.
2. The hydrological characteristics of the adjacent matrix for drainage and imbibition cycles.
3. The effective fracture-matrix area for the various transport processes.
4. The characteristics of the network of fractures, particularly its spacing, connectivity, and the distribution of fracture permeabilities.

In present models of repository behavior, the practice currently followed for items (1) and (2) involves assigning van Genuchten parameters to match available field data or (rather sparse) laboratory data on saturation and capillary pressures (Bodvarsson et al., 1997). This approach allows for a convenient parametric representation, but is not justified from first principles (van Genuchten models were developed for drainage in soils, and may not necessarily apply to tuff or fractures or to imbibition processes). In fact, a Brooks and Corey representation, which is computationally simpler, can be used with equal justification. To our knowledge, the fracture hydrologic parameters have not been measured, but are assigned from matching field data (Bodvarsson et al., 1997; see also discussion on parameter identification below). Sonnenthal et al. (in Bodvarsson et al., 1997) proposed an indirect method, in which the variability of permeability values from pneumatic testing field data is mapped to that of mean fracture aperture, which is subsequently used to infer a van Genuchten parameter. Although based on a number of assumptions, this indirect approach can be useful and needs to be pursued further. Identifying the spatial correlation structure of fracture apertures is also important and needs to be pursued as well. In this direction, the work of Glass et al. (1996, 1997) should be useful.

Measurements of the hydrologic properties of the matrix, particularly of capillary pressure, have been conducted. It is obvious, however, that additional data are needed, particularly for relative permeabilities in imbibition and drainage, to minimize the number of parameters indirectly estimated from matching field data. Finally, an effort needs to be launched to study what effect pore-lining minerals at the fracture-matrix interface, resulting from precipitation, or their removal, resulting from dissolution reactions, will have on imbibition and diffusion into the matrix.

The effective fracture-matrix area (item (3) above) has not been independently measured or characterized. In fact, previous site-scale models (Bodvarsson and Bandurraga, 1996) did not account for such correction, even though early experimental evidence (e.g. Nicholl et al., 1992) was suggestive of a reduced area of contact. The need for a (large) reduction factor has been necessitated from the recent revised estimates of higher infiltration, which apparently can only be reconciled by an increased flow in the fracture network. Bodvarsson et al. (1997), Robinson et al. (1997) and Ho (1997) have proceeded with incorporating such a reduction factor in their studies. In current practice, the fingering pattern in the fracture (which is the origin of the reduction factor) is essentially ignored, in that standard continuum equations are used for the displacement in the fracture (using the same van Genuchten formulation for relative permeabilities and capillary pressure, regardless of flow rates, fracture orientation, etc). It should be apparent from the previous discussion that if at all, the latter would be applicable only for conventional, capillary-controlled displacement in random media, and certainly not when Ca and B are relatively large, or in cases where the fracture aperture is spatially correlated over large scales, either of which will create a channelized displacement. Despite this inconsistency, the reduction factor is used in conjuction with the standard formalism. Three different options have been considered, where the reduction factor is: (i) constant, (ii) proportional to a power of the liquid saturation in the fracture, (iii) equal to the relative permeability of the liquid in the fracture. The current consensus is that the latter option actually leads to a better match of the hydrologic field data. It must be noted that such a reduction factor will lead to an effective fracture-matrix area of interaction which can be 1000 times smaller than the geometric.

The importance of a small effective fracture-matrix area reflects the need to increase *substantially* the flow partitioned in the fracture. In essence, this is another admission of the existence of *fast paths*. Although only recently acknowledged, a reduced fracture-matrix area has a well-based physical justification, as discussed. The currently used option, based on relative permeability, however, is ad hoc and not readily justifiable. In fact, a reduction factor based on saturation is more consistent with the actual physics (although in a displacement in a prewet fracture wetting films will cover the fracture surface and may further increase the area of interaction). A recommendation for a more consistent approach is given in a later section. In defense of the approach taken, it must be pointed out that the reduction factor in coarse-grid numerical models, typically used in Yucca Mountain site-scale models, is actually an overall factor that incorporates in one parameter the combined uncertainty about the overall matrix-fracture geometry over the grid block volume, which contains several fractures. This point will be further discussed below.

With respect to item (4) above, little is known about the properties of the fracture network. Overall fracture permeabilities have been inferred from pneumatic tests, while outcrop fracture maps have also been traced (for a recent application, see Eaton et al., 1996). Current simulation practice, however, is based on the assumption of a well-connected, isotropic continuum with uniform permeabilities. In reality, one expects that due to orientation, the fracture network will actually be anisotropic, that the relative permeabilities and the flow pattern in horizontal fractures will be different than in vertical, and specifically, that patterns along horizontal fractures will be less or not at all channeled or fingered, hence the effective fracture-matrix area will also be different in different directions. An improvement of the simulation to account for these differences should be considered. Distributing permeabilities in the fracture network will result in enhanced dispersion of flow paths and should also be attempted. We note the effort to use geostatistics in the distribution of zeolite abundance, in the recent work of Robinson et al. (1997), and we believe that this approach should also be extended to the permeabilities of matrix and fracture networks.

(iii). Numerical Simulation

Currently, the simulation of the fracture-matrix interaction is handled differently, depending on the application: For the thermal-hydrologic response, due to excessively large computational requirements, use is made of the Effective Continuum Model (ECM), which proceeds with the assumption of capillary, thermal and chemical (namely mass diffusion) equilibrium between matrix and fracture, and considers the system as an equivalent continuum (for a recent thermal-hydrologic application, see Birkholzer and Tsang, 1997). For the case of species mass transport under isothermal conditions, a dual permeability (DK) model is used, in which two effective continua (the matrix and the fracture) coexist at each grid point.

Due to computational restrictions and the large-scale nature of the problem, computational grids are necessarily coarse, the typical grid block containing a multitude of fractures (see, for example, the schematics of Figure 3 reprinted from Glass et al., 1996). Advances in computational capabilities (parallel processing, for example) will lead to further reduction in grid block size. For instance, 3-D site transport models with grid block size of 50 m are now possible (Zyvoloski et al., 1997). Nonetheless, existing computer models are effectively *volume-averaging* processes oocuring over a large number of fractures, inherently containing a number of fracture-matrix interactions. For linear diffusion processes (such as molecular species and thermal energy at conditions of saturated flow) volume-averaging is relatively straightforward, and would result (for the case of the DK model) into defensible effective transport coefficients between fracture and matrix. Then, the arguments used above (and Figure 2, for example) will carry over, with appropriate geometric modifications, to the larger scale as well. However, this is not the case for two-phase flow, such as imbibition, drainage or counter-current flow, which are non-linear processes, and the averaging of which is not straightforward (particularly when capillary-end effects and capillary barriers are involved, see also Yortsos et al., 1993). In current practice, the large-scale interaction between fracture and matrix continua for unsaturated flow (for instance, in the DK model) is approximated by an effective transport coefficient, which lumps all underlying interactions, including unstable flow, the matrix-fracture effective area, capillary discontinuities, etc., into effective transport parameters coupling fracture and matrix continua. At present, this averaging process is, at best, empirical, and efforts should be made to improve its state. The same applies to the heat-pipe problem, where flows are counter-current.

The shortcomings of ECM have been addressed in previous studies (e.g. Witherspoon et al., 1996). Using the above formulation, we can delineate its applicability as follows. For equilibrium to be reached within a matrix block of linear size l, requires a characteristic time of the order of

$$t_{char} \sim l^2 / D \tag{9}$$

where D is the diffusivity appropriate to the quantity being transported (molecular species, thermal energy or capillarity) and we have assumed no reduction in the fracture-matrix area. For $l = 1$ m, this time may range between 10^6 sec (~ 10 days) to 10^{10} sec (~ 300 years), for heat conduction to mass diffusion, respectively (and where we used the previous values for diffusivities). Capillary diffusion-imbibition will fall in-between these two extremes. Now, for equilibrium between matrix and fracture to be valid, the advective flux in the fracture must be sufficiently small, so that the advected quantity has not been transported over distances larger than the matrix linear size over the same time. Otherwise stated, this implies that the Peclet number, $Pe_{i,f}$, is of order 1. (The same can also be deduced from Figure 2, where fracture-matrix equilibrium requires reaching the plateau on the rightmost part of the curve. In fact, Nitao's (1992) condition, $q^* \sim D_c$, is also equivalent to the same condition and to $Pe_{c,f} \sim 1$, if one notes that in his definition, q^* is actually

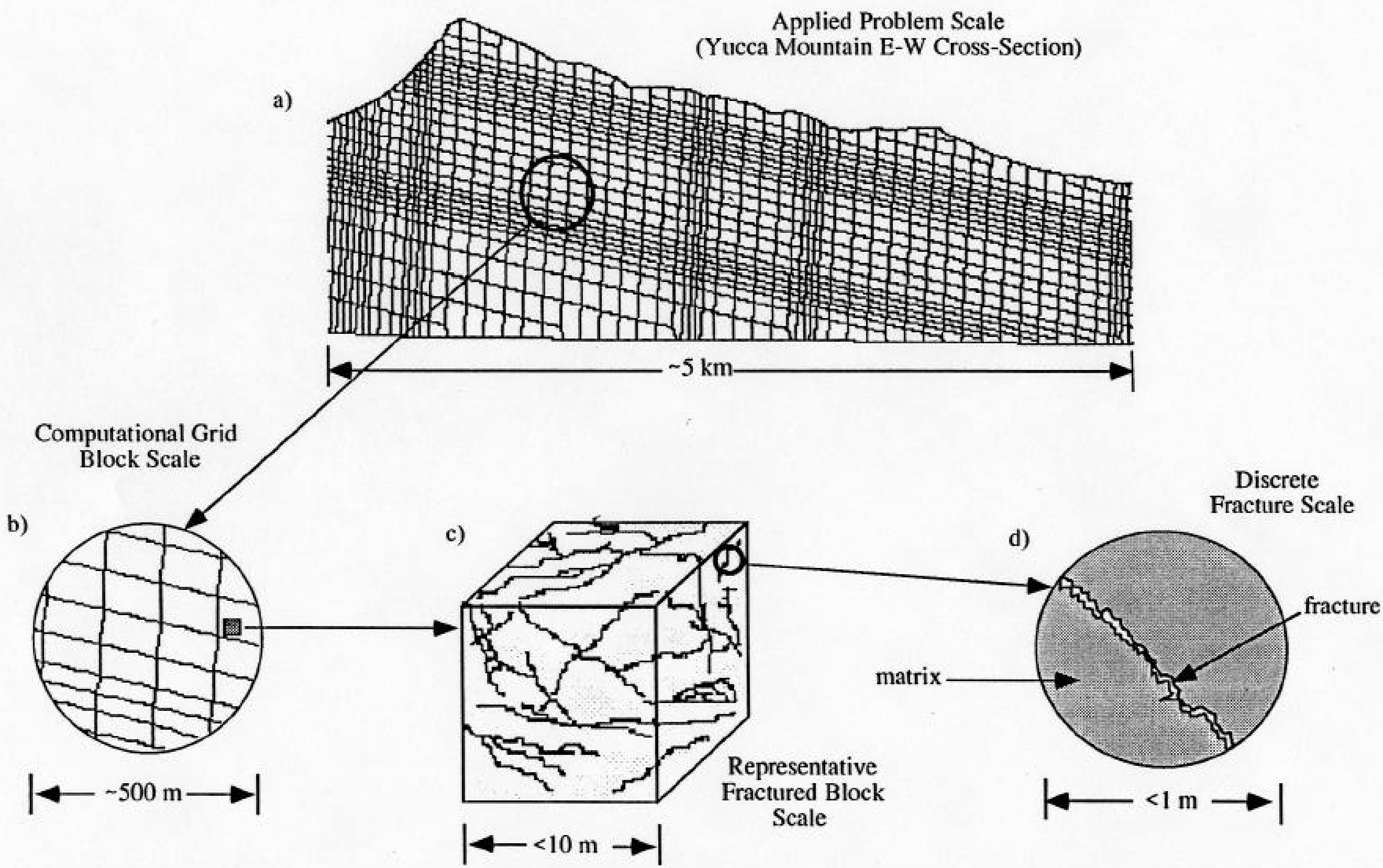

Figure 3: Averaging inherent in the use of equivalent continua models: It is neither possible nor desirable to model large field problems (a) at the scale of individual fractures (d). It is however, essential that numerical models be formulated in a manner that is consistent with the behavior of individual fractures (d) and fracture networks (c). Several discrete scales of averaging for both material properties and physical processes may be required to move from the scale of a single fracture (d) to that of a computational grid block (b).

01_fracture to grid

the product *ql.)* This leads to estimates for the maximum flow velocity in the fracture of the order of 10^{-4} cm/sec (~ 3.3x 10^{3} cm/year) to 10^{-8} cm/sec (~ 0.33 cm/year), in the respective cases, for conditions of fracture-matrix equilibrium. Current infiltration estimates are of the order of mm/year. Given, however, that flow is significantly partitioned in the fractures, and the effect of the reduced fracture-matrix interface, these limits are likely to be exceeded, at least for the case of slow diffusive transport (namely for mass diffusion or for imbibition in a tuff of small permeabilities). On the other hand, fracture-matrix equilibrium should be possible for thermal energy or for the imbibition of a high permeability matrix. The inadequacy of ECM to capture transient events of high infiltration rates was recently documented in the Fran Ridge field test (Eaton et al., 1996).

In an effort to salvage ECM, a modification was recently proposed (Ho, 1997) that effectively forces more fluid in the fracture than allowed from the original model. In this approach, the maximum water saturation in the matrix, termed the "satiated water saturation", S_{sm}, is not set equal to one (as currently used), but becomes instead an adjustable parameter. By reducing this parameter, more flow is effectively allocated to the fracture, thus mimicking the effect of an area reduction factor. Physically, S_{sm} can be related to the trapped non-wetting phase (air in the present case) saturation, S_{nwr}, during an imbibition process, through

$$S_{sm} = 1 - S_{nwr} \tag{10}$$

In quasi-static imbibition, the trapped saturation $Snwr$ is well-defined and can be related to the pore-structural parameters of the porous medium. In fact, in the analogous problem of waterflooding a water-wet oil reservoir, S_{nwr} is the residual oil saturation, typically of the order of 0.3, which is the target of many enhanced recovery methods. In the present context, the situation may not be entirely analogous, in that trapped air may slowly dissolve in water, if the latter is not saturated, and another diffusion process may need to be considered. Nonetheless, we believe that the concept is worth studying, and, in fact, it should not be restricted to the ECM formalism alone.

In their current van Genuchten version, all site-scale models assume $S_{nwr} = 0$. In general, we expect that S_{nwr} would be a function of Ca (as well as B, in the case of gravity instabilities). High-rate imbibition in the absence of gravity instability would result in a more uniform displacement, with accordingly lower S_{nwr}. Gravity instabilities would lead to effectively higher trapped non-wetting phase saturation. In addition, large-scale averaging, implicit to the coarse grids of the Yucca mountain project, leads to *large-scale trapping* (Yortsos et al., 1993), namely to macroscopically trapped saturations due to bypassing of macroscopic regions. In the context of a naturally fractured medium, this could be due to either trapped fractures or partially saturated matrix blocks. This trapping would also result in a non-zero effective S_{nwr}. It follows that non-vanishing S_{nwr} should be considered in the relative permeability and capillary pressure formalisms for imbibition in the various models (TOUGH and FEHM), regardless of the mode by which they operate (ECM or DK). Such a modification can conceivably lead to more reasonable and defensible (e.g. based on fracture saturation) reduction factors. Whether, however, it would also lead to an improvement of the performance of the ECM model remains to be seen, since in comparing ECM with DK, the effect of a reduced S_{sm} should be about the same in both models.

The transport problem in the unsaturated zone below the repository and further into the water aquifer, has less severe computational demands and can be modeled by the dual permeability (DK) model. To account for the great disparity in travel times in the fracture and matrix (see equation (2)), Robinson et al. (1997) proposed a particle tracking approach, which appears to improve dramatically the computational requirements. At present, this approach is best suited for 1-D computations, however, and efforts should be made to modify it for the more challenging 3-D site-scale problem. A variant of the same method could also be considered for the imbibition problem, which shares common diffusive aspects with molecular diffusion (assuming, of course, that all other pertinent aspects of imbibition are kept under consideration).

We conclude with a comment on parameter estimation. The existing computer models have been used in an "inverse" mode to estimate parameter values by matching field data using an optimization algorithm. Bodvarsson et al. (1997) describe this approach in considerable detail. Geothermal temperature data have also been used for an indirect estimate of the percolation flux. Work along these directions is needed and these efforts should continue. At the same time, it must be pointed out that the inverse algorithm is inherently non-unique, limiting the confidence on the estimates so obtained. Furthermore, the estimation is usually done by matching field data to predictions from a model run in an 1-D mode. This effectively diregards lateral flow or transport and adds uncertainty to the relevance of the estimates so obtained. It is somewhat disconcerting, in this context, that in order to reconcile, using the present methodology, available hydrologic data with the new rain infiltration estimate, a *structural* change in the model (namely the introduction of the effective fracture-matrix interaction), was necessary. As pointed out above, in many instances this required a reduction factor of the order of 1000. In retrospect, this reduction (although not of this magnitude) being physically justifiable, should have been used before. In fact, a consideration of the effect of instabilities in the flow in fractures (although not an explicit reduction of the fracture-matrix area) was clearly pointed out in the work of Glass et al. (1996) and recommended in recommendation No. 15c of Witherspoon et al. (1996).

Conclusions and Recommendations

A good description of the fracture-matrix interaction is necessary to reduce uncertainties in the numerical predictions of the repository performance and in process assessment, in general. In many cases, this interaction takes the simple form of a competition between advection in the fracture network and diffusion (mass, heat, capillarity) in the matrix. The partition of flow between fracture and matrix is dictated by parameters such as the capillary diffusivity (imbibition), the area of interaction and the amount of maximum trapped saturation of the non-wetting phase (air) in the grid block volume. Reaching conditions of fracture-matrix equilibrium is controlled by the magnitude of the diffusivity, the flow rate partition and the time elapsed. In typical applications, fracture-matrix equilibrium is likely for thermal energy and for the imbibition of a high-permeability matrix, but unlikely for mass diffusion and the imbibition of a low-permeability tuff. The latter is common to many rocks of the Yucca mountain. In such cases, the assumption of equilibrium is likely to fail. In the current coarse grid simulation, the representation of this interaction is through effective parameters, notable among which is the effective area of fracture-matrix interaction, expressed through a reduction factor that reflects the limited contact resulting from channelized fracture flow. To match field data, reduction factors as low as 10^{-3} have been postulated. This is a drastic departure from previous simulation practice, where this concept was not used. Additional uncertainty, particularly for two-phase flow processes (imbibition, drainage and heat pipes), is introduced due to the volume-averaging over a number of fracture-matrix areas, inherent to the coarse description.

Main recommendations that may help reducing this uncertainty include:

1. <u>Revisit the concept of reduction factor</u>.

Use the experimental information reported in Glass et al. (1997) and earlier publications, on displacement patterns at various conditions, to estimate reliably the effective area (and the corresponding reduction factor). Then, account for a possible increase of the factor due to the stabilization of the displacement exerted by imbibition in the matrix. Modify the fracture hydrological parameters, particularly the relative permeabilities, to account for channelized displacement, by considering rate and gravity effects where appropriate. Allow for anisotropy in permeability, displacement and reduction factor in the fracture continuum in the horizontal and vertical directions.

2. Allow for the possibility of non-zero trapped (residual) air saturation.

Account for non-zero trapped saturation in the various lithological units, by considering the direction (imbibition) and rate of invasion. Consider the effect of large-scale trapping, due to large-scale heterogeneity in the grid block, in increasing the effective residual gas saturation. Non-zero values may lead to lower, and thus more defensible, reduction factors.

3. Improve the estimation procedure for matching field hydrologic data.

Analyze the limitations of the 1-D model (only vertical flow) currently used to match field data and estimate parameters. Allow for the possibility of lateral flow, due to capillary and flow barriers, anisotropy, etc. Study the consequences of non-uniqueness inherent to the inversion process.

4. Improve the large-scale description of two-phase flow processes.

Revisit the formalism for representing unsaturated flow in a grid block, by accounting for effective large-scale permeabilities, relative permeabilities, capillary pressures, large-scale trapped saturations and the fracture-matrix interaction. In this context, particular attention needs to be payed to the heat pipe description in this context. Consider the extension of the particle-tracking algorithm to 3-D and to other diffusive processes.

5. Justify the use of ECM for TH predictions.

Carefully delineate the validity of capillary equilibrium in ECM applications. Revisit the ECM formalism and validity in light of 1 and 2 above. Revisit the heat pipe representation.

Other recommendations are listed in the text.

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APPENDIX B: COMMENTS ON WASTE ISOLATION STUDY

In the course of its review of the development of the TSPA-VA, the PAPR Panel reviewed the *Waste Isolation Study*, B00000000-01717-5705-00062 REV 2 (May 13, 1997).

Although this report is in a draft stage, the Panel was concerned about some of the statements made and the approaches used. The more significant comments and observations of the Panel are summarized below.

1. During the meeting of the NWTRB Panel on Environmental Regulations (October 21, 1997), the DOE representative was careful to point out that what some people refer to as the DOE "interim standard" is not correct. He emphasized that DOE does not set standards, that what they have proposed for use is more properly referred to as an "interim post-closure performance measure," and that it was developed solely to help guide the DOE technical program. The PAPR Panel agrees that this is an important distinction. Yet, the performance measure is referred to as a "standard" throughout the Waste Isolation Study. The same error is made in the TSPA-VA "Methods and Assumptions" document (B00000000-01717-2200-00193, August 13, 1997).

2. In making decisions on which additional engineered barriers may be justified, the analysts state that (1) they will consider only those that fall within a specific cost limitation; and that (2) this approach is in accordance with the ALARA criterion. The PAPR Panel questions these statements for the following reasons:

   a) Normally an ALARA cost limitation (see, for example, 10 CFR Part 50, Appendix I, USNRC, 1976) is based on how much the collective dose to the neighboring population can be reduced as a result of a given additional expenditure to implement more effective control measures; it is not based on a percentage of the total cost of a project;

   b) Under the standard guidance on radiation protection (ICRP, 1991), the first objective is to assure that the dose rate limits are met. The ALARA criterion is applied only after this goal has been met, the purpose being to determine if dose reductions below the limits are economically justified.

The Panel believes that this portion of the Waste Isolation Study needs to be re-evaluated.

3. At the time the report was prepared, DOE had included the EPA Standards for Ground Water Protection (U.S. EPA, 1996) as a part of its interim performance measure. Although the Panel now understands that this is no longer the case, the need to protect groundwater may still be included in the standards for the proposed high-level waste repository at Yucca Mountain. Although the existing EPS Ground Water

Standards specify a limit of 5 pCi/l for ^{226}Ra and ^{228}Ra, the limit for other alpha emitting radionuclides is 15 pCi/l. For this reason, and to enable DOE to be in a position to comment on whatever regulatory requirements may be imposed, the Panel recommends that the DOE staff review the EPA Ground Water Standards in detail and:

a) Estimate the dose rate limits the Standards would impose for the key radionuclides that may be released from the proposed repository;

b) Determine whether the dose rate limit on multiple pathways, or the limits on individual radionuclides, will govern and under what conditions; and

c) Identify those cases for which the 4 mrem/y dose rate limit from man-made beta and gamma emitting radionuclides will prevail.

4. One of the radionuclides cited (page 3-13) as being a "primary contributor to dose" is ^{129}I. The NCRP (Report No. 80, 1985, page 41) has concluded that the published information suggests "that ^{129}I does not pose a meaningful threat of thyroid carcinogenesis in people." It would appear useful to review similar background information on the detailed physical, biological, and chemical information on each of the other radionuclides currently on the list of those considered important by the TSPA-VA team.

5. The comparative evaluations of the various cases and barriers are helpful. Nonetheless, the presentation of the results in several cases could be made more clear. For example:

   a) The meaning of the negative numbers in the third column of Table 3-4 needs to be explained;

   b) The information on BDCFs presented just below Table 3-5 would be improved if a column were added to indicate the BDCF for drinking the water;

   c) The title of Table 3-6 fails to mention that the quoted values are for "drinking water" and that they are expressed as "dose rates," not "doses"; and

   d) Table 4-1 could be improved through the addition of a column indicating the "APF" for each barrier.

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APPENDIX C: PEER REVIEW PANEL

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ACRONYMS AND ABBREVIATIONS

CFR	Code of Federal Regulations
CRM	corrosion resistant metal
CRWMS	Civilian Radioactive Waste Management System
DCF	Dose Conversion Factor
DHLW	Defense High Level (radioactive) Waste
DOE	U.S. Department of Energy
DKM	dual permeability model
DQO	data quality objective
EBS	Engineered Barrier System
ECM	equivalent continuum model
ECRB	Enhanced Characterization of the Repository Block
Eh	oxidizing potential
EPA	U.S. Environmental Protection Agency
ESF	Exploratory Studies Facility
HLRW	high-level radioactive waste
ICRP	International Commission on Radiological Protection
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
M&O	Management and Operating Contractor
MIC	microbially induced corrosion
MTHM	metric tons heavy metal
NCRP	National Council on Radiation Protection and Measurements
NWTRB	Nuclear Waste Technical Review Board
pH	measure of the hydrogen ion concentration or level of acidity
PSHA	probabilistic seismic hazard analysis
PTn	Paintbrush nonwelded tuff layer
PVHA	probabilistic volcanic hazard analysis
RBE	(first use, page 58, need spelling here and there)
SCC	stress corrosion cracking
SNF	spent nuclear fuel
SZ	saturated zone
THCM	thermo-hydro-chemical-mecanical
TSPA	Total System Performance Assessment
TSPA-95	TSPA completed in 1995
TSPA-VA	TSPA supporting the Viability Assessment
TSw	Topopah Spring welded tuff layer
USGS	U.S. Geologic Survey
USNRC	U.S. Nuclear Regulatory Commission
UZ	unsaturated zone
VA	Viability Assessment
WF	waste form
WIPP	Waste Isolation Pilot Plant
WP	waste package

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